

10712258 09/20/05

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1626KAS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 JUL 20 Powerful new interactive analysis and visualization software,
STN AnaVist, now available
NEWS 4 AUG 11 STN AnaVist workshops to be held in North America
NEWS 5 AUG 30 CA/CPlus - Increased access to 19th century research documents
NEWS 6 AUG 30 CASREACT - Enhanced with displayable reaction conditions
NEWS 7 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY
NEWS 8 SEP 22 MATHDI to be removed from STN

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 15:12:04 ON 01 OCT 2005

FILE 'REGISTRY' ENTERED AT 15:12:52 ON 01 OCT 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

10712258 09/20/05

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 SEP 2005 HIGHEST RN 864353-93-5
DICTIONARY FILE UPDATES: 30 SEP 2005 HIGHEST RN 864353-93-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

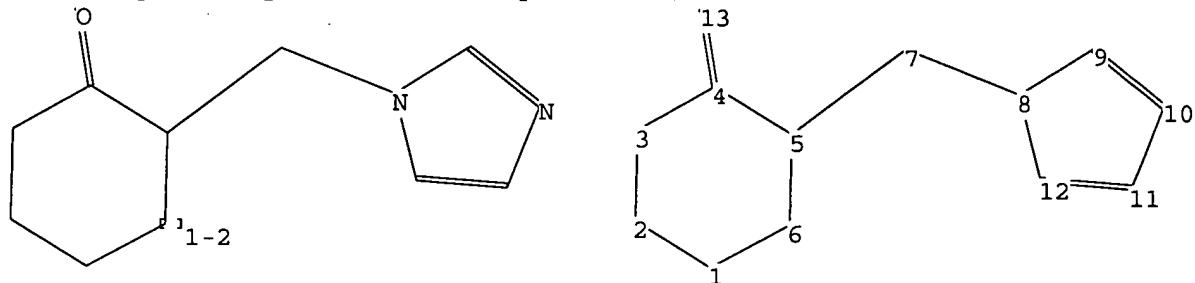
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10712258.str



chain nodes :

7 13

ring nodes :

1 2 3 4 5 6 8 9 10 11 12

chain bonds :

4-13 5-7 7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-13 5-6 7-8 8-9 8-12 9-10 10-11

exact bonds :

5-7 11-12

isolated ring systems :

containing 8 :

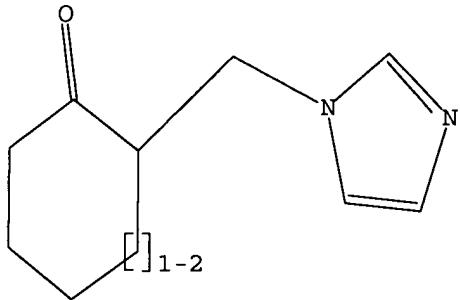
10712258 09/20/05

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11
SAMPLE SEARCH INITIATED 15:13:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 496 TO ITERATE

100.0% PROCESSED 496 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8584 TO 11256
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 15:13:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9119 TO ITERATE

100.0% PROCESSED 9119 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.01

L3 24 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
161.33 161.54

FILE 'CAPLUS' ENTERED AT 15:13:25 ON 01 OCT 2005

10712258 09/20/05

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 1 Oct 2005 VOL 143 ISS 15

FILE LAST UPDATED: 30 Sep 2005 (20050930/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 22 L3

=> s 14 and oxazolidine
 3939 OXAZOLIDINE
 1268 OXAZOLIDINES
 4294 OXAZOLIDINE
 (OXAZOLIDINE OR OXAZOLIDINES)
L5 2 L4 AND OXAZOLIDINE

=> d ibib abs hitstr tot

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:652673 CAPLUS

DOCUMENT NUMBER: 141:174173

TITLE: Process for the preparation of imidazolyl compounds
INVENTOR(S): Verbeek, Jan-Maarten; Van der Meij, Paulus F. C.
PATENT ASSIGNEE(S): Solvay Pharmaceuticals B.V., Neth.

SOURCE: U.S. Pat. Appl. Publ., 6 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

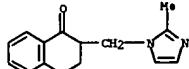
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004158077	A1	20040812	US 2002-712258	20031114
PRIORITY APPLN. INFO.:			EP 2002-79038	A 20021118
			NL 2002-1021939	A 20021118

OTHER SOURCE(S): MARPAT 141:174173

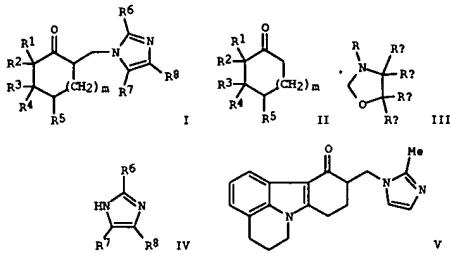
GI

current application

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 stirred for 3 h at 120° C to afford V.HCl in 77% yield. The method is esp. useful for the prepn. of selective neuronal 5-HT receptor antagonists, which are useful as anti-migraine and antipsychotic agents.
 IT 697807-10-6
 RL: IMP (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of imidazolyl compds.)
 RN 697807-10-6 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(2-methyl-1H-imidazol-1-yl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl



AB The invention discloses a method for the preparation of imidazolyl compds., such as I (R1, R3 = alkyl, alkoxyalkyl, optionally substituted aryl or heteroaryl; R1R3 = fused homocyclic or heterocyclic system comprising one or more rings; R2, R4 = H, double bond (optionally part of an aromatic system); R3 = H, alkyl, alkoxy, alkoxyalkyl, halogen; R4, R5, R6, R7, R8 = H, alkyl; m = 1 - 2; R6 = H, alkyl, acid addition salts), by reacting a cyclic ketone of formula II with an oxazolidine derivative III (R = H, alkyl optionally substituted with OH or an optionally substituted aryl group; Ra, Rb, Rc, Rd = H, alkyl), followed by reaction with an imidazole IV. Thus, 5,6,9,10-tetrahydro-4H-pyrido[3,2,1-kl]carbazol-11(8H)-4-one and MeSO3H in BuOH were heated to 70° C and then treated with 3-oxazolidinethanol in BuOH, and the mixture was heated for 50 min at 80° C. Then, 2-methylimidazole in BuOH was added and the mixture was heated for 50 min at 80° C. Then, 2-methylimidazole in BuOH was added and the mixture was

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:453190 CAPLUS

DOCUMENT NUMBER: 141:23529

TITLE: Novel process for the preparation of imidazolyl compounds, particularly ondansetron, cilanstetron, and analogs, using oxazolidine derivatives as formaldehyde equivalents in a Mannich-like reaction

INVENTOR(S): Verbeek, Jan-Maarten; Van Der Meij, Paulus F. C.
PATENT ASSIGNEE(S): Solvay Pharmaceuticals B.V., Neth.

SOURCE: PCT Int. Appl., 22 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 200406116	A1	20040603	WO 2003-EP50841	20031117
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HP, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GE, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
CA 2504614	AA	20040603	CA 2003-2504614	20031117
EP 1565445	A1	20050824	EP 2003-811396	20031117
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: EP 2002-79038 A 20021118
WO 2003-EP50841 W 20031117

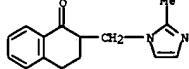
OTHER SOURCE(S): CASREACT 141:23529; MARPAT 141:23529

GI

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 as anti-migraine and antipsychotic agents, e.g., ondansetron and cilanstetron. The method is superior to prior art Mannich processes using formaldehyde, which give tar-like byproducts when scaled up. For instance, 1,2,3,9-tetrahydro-9-methyl-4H-carbazol-4-one and MeSO3H in BuOH were heated to 90° and then treated with 3-oxazolidinethanol in BuOH, and the mixt. was heated for 50 min at 80°. Then, 2-methylimidazole in BuOH was added and the mixt. was stirred for 2 h at 120°. Extn. and crystn. gave V.HCl, i.e. ondansetron HCl, in 70.1% yield and ≥ 95% purity, with an addnl. 14.5% product in the mother liquor. Similar preps. of (+)-cilanstetron HCl and another compd. are also given.

IT 697807-10-6
 RL: IMP (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (target compound; improved preparation of imidazole 5-HT antagonists (ondansetron and cilanstetron) using oxazolidine derivs. as formaldehyde equivalent in Mannich-like reaction)

RN 697807-10-6 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(2-methyl-1H-imidazol-1-yl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to an improved method for the preparation of imidazolyl compds. I (wherein: Ra, Rb = C1-C6 alkyl, C1-C6 alkoxyalkyl, optionally substituted aryl or heteroaryl; or RaRb = fused homocyclic or heterocyclic system comprising one or more rings; Ra'Rb' = H2, carbon-carbon double bond (optionally part of an aromatic system); Rc = H, C1-C6 alkyl, C1-C6 alkoxy, C1-C6 alkoxyalkyl, or halogen; Rd = H or C1-C4 alkyl; Re = H or C1-C4 alkyl; m = 1 or 2; R1 = H or C1-C4 alkyl; as well as acid addition salts). The method is characterized in that a cyclic ketone of formula II reacts with an oxazolidine derivative III, followed by reaction with an imidazole IV, optionally followed by reaction with a suitable acid (wherein: R1, Rd, and Re = as given above; R = H, C1-C4 alkyl optionally substituted with OH or an optionally substituted aryl group; R', R'', R''', and R'''' = H or C1-C4 alkyl). The method is especially useful for the preparation of selective neuronal 5-HT receptor antagonists, which are useful

Page 5 SAEED

10712258 09/20/05

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
--	---------------------	------------------

FULL ESTIMATED COST	13.12	174.66
---------------------	-------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
--	---------------------	------------------

CA SUBSCRIBER PRICE	-1.46	-1.46
---------------------	-------	-------

STN INTERNATIONAL LOGOFF AT 15:15:23 ON 01 OCT 2005